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SYSTEMS, METHODS AND COMPUTER PROGRAM PRODUCTS FOR DETERMINING PARAMETERS FOR CHEMICAL SYNTHESIS AND FOR SUPPLYING THE REAGENTS, EQUIPMENT AND/OR CHEMICALS SYNTHESIZED THEREBY

Field of the Invention

This invention relates to data processing systems, methods and computer program products, and more particularly to systems, methods and computer program products for chemical synthesis.

Background of the Invention

Chemicals are synthesized for various applications in commercial and academic environments. In chemical synthesis, a plurality of reagent chemicals are used to synthesize a target chemical, by reacting the reagent chemicals in predefined equipment according to a predefined procedure. The reagent chemicals, the target chemical, the equipment and the procedure provide the parameters for chemical synthesis.

The identification of the reagent chemicals, the equipment and the procedures to synthesize the target chemical may be contained within laboratory notebooks that are maintained by a commercial or academic organization. Moreover, the open literature also contains many references that can identify reagent chemicals, equipment and procedures that can be used to synthesize a target chemical. As one example, see Wolfe et al., *Highly Active Palladium Catalysts for Suzuki Coupling Reaction*, J. Am. Chem. Soc., Vol. 121, 1999, pp. 9550-9561. In the "Experimental Section" of this publication, various procedures are described for synthesizing aryl halides.

Unfortunately, it may be difficult to find an appropriate procedure for synthesizing a desired target chemical, and it also may be difficult and/or time consuming to identify and procure the reagent chemicals and/or equipment that are used to synthesize the desired target chemical.

Summary of the Invention

Embodiments of the present invention comprise systems, methods and computer program products for determining parameters for chemical synthesis in response to a user query that identifies a target chemical. In response to the user identification of the target chemical, a listing is displayed of reagent chemicals that are used to synthesize the target chemical. A listing also is displayed of equipment that is used to synthesize the target chemical. A listing also is displayed of a procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure.

In other embodiments, user input is accepted to electronically order the reagent chemicals that are used to synthesize the target chemical, the target chemical itself, and/or the equipment that is used to synthesize the target chemical. In response, a transaction is performed to electronically order the reagent chemicals that are used to synthesize the target chemical, the equipment that is used to synthesize the target chemical and/or the target chemical itself.

In yet other embodiments, prior to accepting a user identification of a target chemical, a database is populated with a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals, a plurality of corresponding listings of equipment and a plurality of corresponding listings of procedures. The database then is searched in response to a user identification of a target chemical. Thus, in embodiments of the present invention, target chemicals, their reagent chemicals, their equipment and their synthesis procedures may be entered into a database and may be queried by a user. Once identified, the reagent chemicals, the target chemicals, and/or the equipment may be electronically ordered.

It will be understood that various combinations of data entry, user queries and transactions that were described above also may be provided according to embodiments of the present invention. Thus, for example, user identification of the target chemical may be provided to a preexisting database that can display a listing of reagent chemicals, a listing of equipment and a listing of a procedure. Moreover, a database may be provided which comprises a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals, a plurality of corresponding listings of equipment and a plurality of corresponding listings of procedures. Alternatively, reagent chemicals that are used to synthesize a target chemical and/or equipment that

is used to synthesize a target chemical may be ordered from an electronically displayed listing of the reagent chemicals, the equipment and the procedure, in response to user input. Other subcombinations also may be provided.

Brief Description of the Drawings

Figures 1A-1G are block diagrams of systems, methods and/or computer program products according to embodiments of the present invention.

Figure 2 is a diagram of computer systems that can practice methods and/or include computer program products according to embodiments of the present invention.

Figure 3 is a flowchart of data entry according to embodiments of the present invention.

Figures 4-14 illustrate displays that may be used for data entry according to embodiments of the present invention.

Figure 15 is a flowchart of entering properties according to embodiments of the present invention.

Figure 16 illustrates a display that may be used to enter a reference according to embodiments of the present invention.

Figure 17 is a flowchart of operations for performing user queries according to embodiments of the present invention.

Figures 18 and 19 illustrate displays that may be used for performing queries according to embodiments of the present invention.

Figures 20 and 21 illustrate displays of listings of reagent chemicals, equipment and procedures according to embodiments of the present invention.

Figure 22 is a flowchart of scaling of listings according to embodiments of the present invention.

Figure 23 is a flowchart of transactions according to embodiments of the present invention.

Detailed Description of Preferred Embodiments

The present invention now is described more fully hereinafter with reference to the accompanying drawings, in which preferred embodiments of the invention are shown. This invention may, however, be embodied in many different forms and should not be construed as limited to the embodiments set forth herein. Rather, these

embodiments are provided so that this disclosure will be thorough and complete, and will fully convey the scope of the invention to those skilled in the art. Like numbers refer to like elements throughout the description of the drawings.

As also will be appreciated by one of skill in the art, the present invention may be embodied as methods, data processing systems, and/or computer program products. Accordingly, the present invention may take the form of an entirely hardware embodiment, an entirely software embodiment running on general purpose hardware or an embodiment combining software and hardware aspects. Furthermore, the present invention may take the form of a computer program product on a computer-usable storage medium having computer-usable program code embodied in the medium. Any suitable computer readable medium may be utilized including hard disks, CD-ROMs, optical storage devices, or magnetic storage devices.

Computer program code for carrying out operations of the present invention may be written in an object oriented programming language such as JAVA®, Smalltalk or C++. The computer program code for carrying out operations of the present invention may also be written in a conventional procedural programming language, such as "C". Microsoft Active Server Pages (ASP) technology and Java Server Pages (JSP) technology may be utilized. Software embodiments of the present invention do not depend on implementation with a particular programming language. The program code may execute entirely on one or more Web servers and/or application servers, or it may execute partly on one or more Web servers and/or application servers and partly on a remote computer (*i.e.*, a user's Web client), or as a proxy server at an intermediate point in a network. In the latter scenario, the remote computer may be connected to the Web server through a LAN or a WAN (*e.g.*, an intranet), or the connection may be made through the Internet (*e.g.*, via an Internet Service Provider).

The present invention is described below with reference to block diagram and flowchart illustrations of methods, apparatus (systems) and computer program products according to embodiments of the invention. It will be understood that each block of the block diagrams and/or flowchart illustrations, and combinations of blocks, can be implemented by computer program instructions. These computer program instructions may be provided to a processor of a general purpose computer, special purpose computer, or other programmable data processing apparatus to produce a machine, such that the instructions, which execute via the processor of the

computer or other programmable data processing apparatus, create structures for implementing the functions specified in the block diagram and/or flowchart block or blocks.

These computer program instructions may also be stored in a computer-readable memory that can direct a computer or other programmable data processing apparatus to function in a particular manner, such that the instructions stored in the computer-readable memory produce an article of manufacture including instructions which implement the function specified in the block diagram and/or flowchart block or blocks.

The computer program instructions may also be loaded onto a computer or other programmable data processing apparatus to cause a series of operational steps to be performed on the computer or other programmable apparatus to produce a computer implemented process or method such that the instructions which execute on the computer or other programmable apparatus provide steps for implementing the functions specified in the block diagram and/or flowchart block or blocks.

In order to provide a complete description of preferred embodiments of the invention in a systematic manner, an overview first will be provided. Detailed embodiments of the invention then will be described.

Overview

Referring now to Figures 1A-1G, block diagrams of systems, methods and/or computer program products according to embodiments of the present invention are shown. In embodiments of Figure 1A, data entry **110** is provided, wherein a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals that are used to synthesize the plurality of target chemicals, a plurality of corresponding listings of equipment that is used to synthesize the plurality of target chemicals and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in the corresponding equipment according to the corresponding procedure, are entered into a database. At Block **120**, a user query that identifies a target chemical is accepted, and a listing of reagent chemicals that are used to synthesize the target chemical, a listing of equipment that is used to synthesize the target chemical, and a listing of the procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, is displayed in response to the

user identification of the target chemical. Finally, at Block **130**, a transaction accepts a user input to electronically order the reagent chemicals that are used to synthesize the target chemical, the target chemical itself and/or the equipment that is used to synthesize the target chemical, and the reagent chemicals, target chemical and/or the equipment is electronically ordered in response to the user input.

As shown in Figures 1B-1D, various combinations of data entry **110**, user query **120** and transactions **130** may be provided according to embodiments of the present invention. Thus, for example, in Figure 1B, data entry **110** is provided to enter into a database, a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals, a plurality of corresponding listings of equipment, and a plurality of corresponding listings of procedures. A user query **120** then may be performed by accepting a user identification of a target chemical, and displaying the corresponding listing of reagent chemicals, equipment and procedure. In embodiments of Figure 1B, transactions need not be performed electronically. Moreover, in Figure 1C, a user query **120** of a preexisting database may be provided wherein, in response to a user identification of a target chemical, a display of a listing of reagent chemicals, a listing of equipment and a listing of a procedure is provided. At Block **130**, a transaction then may be performed to electronically order the reagent chemicals, the target chemical, and/or the equipment. Finally, in Figure 1D, data entry **110** is provided to enter into a database target chemicals, corresponding reagent chemicals, corresponding equipment and corresponding procedures, and then a transaction **130** may be performed from the database without a query.

As also shown in Figures 1E-1G, data entry **110**, user query **120** and transactions **130** may be used separately according to embodiments of the present invention. Thus, in Figure 1E, data entry **110** may be used to populate a database of a plurality of target chemicals, a plurality of corresponding listings of reagent chemicals, a plurality of corresponding listings of equipment and a plurality of corresponding listings of procedures. This database may include three related databases: a chemical database, an equipment database and a supplier database. As part of data entry, a plurality of target chemicals, a plurality of first pointers to a corresponding plurality of listings of reagent chemicals in the chemical database, a plurality of second pointers to a corresponding plurality of listings of equipment in the equipment database, and a plurality of corresponding listings of procedures are entered into the chemical database. The plurality of listings of equipment are entered

into the equipment database, along with a plurality of third pointers to a corresponding plurality of listings of equipment suppliers in the supplier database. The listings of equipment suppliers are entered into the supplier database. This database or databases may be used as was described in Figures 1A, 1B and 1D, and/or for other purposes, such as archival purposes.

As part of data entry, a narrative description of steps of the corresponding procedure may be interactively generated and entered into a database, using the corresponding listing of the reagent chemicals and the corresponding listing of equipment. In particular, user entry of a listing of reagent chemicals that are used in a next step of a procedure to synthesize a target chemical, user entry of a listing of corresponding equipment that is used in the next step, and user entry of the next step may be accepted in response to user indication that the next step is present in the procedure. The target chemical, reagent chemicals, equipment and procedures may be obtained from a publication related to synthesis of the target chemical and/or from proprietary data related to synthesis of the target chemical, for example in lab notebooks.

Moreover, as shown in Figure 1F, user queries **120** of preexisting databases may be performed to accept a user identification of a target chemical and display a corresponding listing of reagent chemicals, equipment and a procedure. In embodiments of user queries, the user may identify the target chemical by formula, chemical structure, chemical compound name and/or CAS number. Moreover, in response to a user query, a listing of target chemicals that match the user query may be displayed, and a user selection of a target chemical from the listing of target chemicals may be accepted. The listing of target chemicals may be prioritized, based, for example, on the extent of match to the user query. The listings of reagent chemicals, equipment and procedures corresponding to the user-selected target chemical then may be displayed. In yet other embodiments, a user identification of a reaction type may be accepted, and a listing of target chemicals that are synthesized using the reaction type may be displayed. A user selection of a target chemical then may be accepted from the listing of target chemicals.

In yet other query embodiments, backward searching may be performed. In particular, a listing of procedures that can be used to synthesize a target chemical may be displayed in response to a user identification of the target chemical. A user selection of a procedure from the listing of procedures may be accepted, and the

listing of reagent chemicals, equipment and the procedure may be displayed in response to the user selection of the procedure. In other query embodiments, forward searching may be performed. In particular, a listing of procedures is displayed that use the target chemical as a reagent chemical, in response to user identification of the target chemical. A user selection of a procedure is accepted. In still other query embodiments, after accepting a user identification of a target chemical, a user selection of a desired quantity of the target chemical is accepted. The listing of the reagent chemicals then is scaled, so as to synthesize the desired quantity of the target chemical. Then, a scaled listing of reagent chemicals, a listing of equipment that is used to synthesize the desired quantity of the target chemical and the listing of the procedure that is used to synthesize the desired quantity of the target chemical is displayed.

Finally, referring to Figure 1G, transactions **130** may be performed independently by electronically ordering the target chemicals, reagent chemicals that are used to synthesize the target chemical and/or equipment that is used to synthesize the target chemical from an electronically displayed listing of the reagent chemicals, of the equipment and of a procedure, in response to user input. In some embodiments of transactions **130**, a kit of reagent chemicals that are used to synthesize the target chemical is ordered. In other embodiments, a kit of the equipment that is used to synthesize the target chemical is ordered. Both kits also may be ordered. In yet other embodiments, the target chemical itself is ordered.

Detailed Embodiments

Some embodiments of the present invention may be practiced on a single computer, for example using a client-server architecture. However, because other embodiments of the present invention may involve storage and/or searching of large numbers of target chemicals and their corresponding reagent chemicals, equipment and procedures, embodiments of the present invention may be implemented on a client-server system, wherein at least one client computer and at least one server computer are connected over a network, such as the Internet.

The Internet is a worldwide decentralized network of computers having the ability to communicate with each other. The Internet has gained broad recognition as a viable medium for communicating and for conducting business. The World-Wide Web (Web) was created in the early 1990's, and is comprised of server-hosting

computers (Web servers) connected to the Internet that have hypertext documents (referred to as Web pages) stored therewithin. Web pages are accessible by client programs (*e.g.*, Web browsers) utilizing the Hypertext Transfer Protocol (HTTP) via a Transmission Control Protocol/Internet Protocol (TCP/IP) connection between a client-hosting device and a server-hosting device. While HTTP and Web pages are the prevalent forms for the Web, the Web itself refers to a wide range of protocols including Secure Hypertext Transfer Protocol (HTTPS), File Transfer Protocol (FTP), and Gopher, and Web content formats including plain text, HyperText Markup Language (HTML), Extensible Markup Language (XML), as well as image formats such as Graphics Interchange Format (GIF) and Joint Photographic Experts Group (JPEG).

A Web site generally comprises a related collection of Web files that includes a beginning file called a "home" page. From the home page, a visitor can access other files and applications at a Web site. A large Web site may utilize a number of servers, which may or may not be different and which may or may not be geographically-dispersed. For example, the Web site of the International Business Machines Corporation (www.ibm.com) includes thousands of Web pages and files spread out over multiple Web servers in locations world-wide.

A Web server (also referred to as an HTTP server) is a computer program that generally utilizes HTTP to serve files that form Web pages to requesting Web clients. Exemplary Web servers include International Business Machines Corporation's family of Lotus Domino® servers, the Apache server (available from www.apache.org), and Microsoft's Internet Information Server (IIS), available from Microsoft Corporation, Redmond, Washington. A Web client is a requesting program that also generally utilizes HTTP. A browser is an exemplary Web client for use in requesting Web pages and files from Web servers. A Web server waits for a Web client, such as a browser, to open a connection and to request a specific Web page or application. The Web server then sends a copy of the requested item to the Web client, closes the connection with the Web client, and waits for the next connection.

HTTP allows a browser to request a specific item, which a Web server then returns and the browser renders. To ensure that browsers and Web servers can interoperate unambiguously, HTTP defines the exact format of requests (HTTP requests) sent from a browser to a Web server as well as the format of responses (HTTP responses) that a Web server returns to a browser. Exemplary browsers that

can be utilized with the present invention include, but are not limited to, Netscape Navigator® (America Online, Inc., Dulles, VA) and Internet Explorer™ (Microsoft Corporation, Redmond, WA). Browsers typically provide a graphical user interface for retrieving and viewing Web pages, applications, and other resources served by Web servers.

As is known to those skilled in this art, a Web page is conventionally formatted via a standard page description language such as HTML, which typically contains text and can reference graphics, sound, animation, and video data. HTML provides for basic document formatting and allows a Web content provider to specify anchors or hypertext links (typically manifested as highlighted text) to other servers. When a user selects a particular hypertext link, a browser running on the user's client device reads and interprets an address, called a Uniform Resource Locator (URL) associated with the link, connects the browser with a Web server at that address, and makes a request (*e.g.*, an HTTP request) for the file identified in the link. The Web server then sends the requested file to the client device which the browser interprets and renders within a display screen.

Referring now to Figure 2, a computer system **210** that can practice methods and/or include computer program products according to embodiments of the present invention, is schematically illustrated. The illustrated system **210** includes a server Web site **212** and a plurality of users, also referred to herein as "customers", who can perform user queries **120** of Figures 1A-1G and/or perform transactions **130** of Figures 1A-1G, and who communicate with the server Web site **212** from customer sites **218** over a computer network, such as the Internet **220**. Customer sites **218** may include a computer display **218a** and a computer **218b**. A pointing device such as a mouse also may be included.

The server Web site **212** includes a Web server **214**, such as a Java Web server, a database server **215** and one or more databases **216**. As shown in Figure 2, the databases **216** may include a chemical database **216a**, an equipment database **216b** and a supplier database **216c**. Other databases also may be provided. Although a single Web server **214** and database server **215** are illustrated, it will be understood that multiple Web servers and multiple database servers (including other application servers) may be utilized according to embodiments of the present invention.

The Web server **214** is the "front end" component of the Web site **212**, and is configured to handle requests from customer sites **218** that access the Web site **212**.

The Web server **214** can include program code, logic and graphics, to interface with the customer sites **218**. Exemplary commercial Web servers that may be utilized as a Web server **214** in the illustrated system **210** are Apache, available from the Apache Server Project, http://www.apache.org; Microsoft's Internet Information Server (IIS), available from Microsoft Corporation, Redmond, Washington; and Netscape's FastTrack® and Enterprise™ servers, available from America Online, Inc., Dulles, Virginia. Other Web servers that may be utilized include Novell's Web Server for users of its NetWare® operating system, available from Novell, Inc., San Jose, California; and IBM's family of Lotus Domino® servers, available from International Business Machines Corporation, Armonk, New York.

As is known by those of skill in the art, a database is a collection of data that is organized in tables or other conventional forms of organization. A database typically includes a database manager and/or database server **215** that facilitates accessing, managing, and updating data within the various tables of a database. Exemplary types of databases that can be used to implement the chemical database **216a**, equipment database **216b**, and supplier database **216c** of the present invention include relational databases, distributed databases (databases that are dispersed or replicated among different points in a network), and object-oriented databases. Relational, distributed, and object-oriented databases are well understood by those of skill in the art and need not be discussed further herein.

The database server **215** operates as a "middleman" server between the Web server **214** and the plurality of databases **216a-216c**. The database server **215** generally includes program code and logic for retrieving data from the databases **216a-216c** (and from sources external to the Web site **212**) in response to requests from the Web server **214**. Commercial database servers that may be utilized as a database server **214** in the illustrated system **210** include Microsoft's SQL server, IBM DB2® Universal Database server, the latter being available from International Business Machines Corporation, Armonk, New York.

Figure 2 illustrates a plurality of databases **216** including a chemical database **216a**, an equipment database **216b** and a supplier database **216c**. However, it will be understood that one or more of these databases may be combined into a single database and that other databases also may be provided at the server Web site **212**.

Data structures of the databases **216a-216c** according to embodiments of the invention now will be described. In embodiments of the invention, the chemical

database **216a** includes listings of a plurality of target chemicals, a plurality of first pointers to a corresponding plurality of listings of reagent chemicals in the chemicals database **216a** that are used to synthesize the plurality of target chemicals, a plurality of second pointers to a corresponding plurality of listings of equipment in the equipment database **216b**, and a plurality of corresponding listings of procedures that are used to synthesize the plurality of target chemicals by reacting the corresponding reagent chemicals in corresponding equipment according to the corresponding procedure. Table 1 provides an example of an architecture of a chemical database **216a** according to embodiments of the present invention.

Table 1: Chemical Database **216a**

ATTRIBUTE	TYPE	DESCRIPTION
name	text	the compound name such as 4-Acetylbiphenyl
id	integer	unique identifier within Table 1
entered_by	text	the runner who input the data
first_entered	timestamp	date/time entry was first entered
modified_by	text	name of last person who modified this record
last_modified	timestamp	date/time entry was last modified
ref	text	the journal references
image_url	text	pointer to the graphic for this compound which is stored on the web server **214**
recipe	text	the protocol text
chemicals	integer[]	first pointers (using the 'id' field) to reagents needed. Points to other records in the chemical database **216a**
equipment	integer[]	second pointers to records in the equipment database **216b**
cas	text	the CAS number
formula	text	the formula
mweight	float8	molecular weight
quantity	float8[]	arrays of integers corresponding to quantity of each equipment
equivalent	float8[]	equivalent of this compound
yield	float8	the yield for this protocol
flask_name	text	the name of the flask used
info	text	keywords
density	float8	density of this compound
bplo	float8	boil point range, low end
bphi	float8	boil point range, high end
fp	float8	flash point
vp	text	vapor pressure
mplo	float8	melting point, low end
mphi	float8	melting point, high end

beilstein	text	beilstein reference
other_names	text	other names
reagents	text	list of the reagents cas#s
smiles	text	structure description
reagent smiles	text	semicolon separated structure descriptions for the reagents
incompatible	text	semicolon separated incompatible chemicals

The equipment database **216b** contains a plurality of listings of equipment that can be used to synthesize various target chemicals. Table 2 illustrates an architecture of an equipment database **216b** according to embodiments of the present invention.

Table 2: Equipment Database **216b**

ATTRIBUTE	TYPE	DESCRIPTION
name	text	name of equipment
id	integer	unique record identifier
suppliers	integer[]	third pointers ('id' value) into the supplier database **216c**
unit	text	measured unit (ml, L, etc.)
our_price	money	our price per unit
om_price	money	average price for outside supplier
size	integer	volume (for flasks)
category 1 = flask 2 = additional equipment 3 = flask equipment	integer	integer describing type of item

The supplier database **216c** contains a listing of suppliers of reagent chemicals and/or equipment. Table 3 is an architecture of a supplier database **216c** according to embodiments of the invention.

Table 3: Supplier Database **216c**

ATTRIBUTE	TYPE	DESCRIPTION
name	text	supplier name (company name)
id	integer	unique record identifier
address1	text	
address2	text	
city	text	
state	text	
website	text	
phone	text	
Index: supplier_id_key	integer	unique record identifier

The server Web site **212** is accessible to customer sites **218** via a computer network such as the Internet **220**. Customers can access the server Web site **212** via a client program, such as a browser and/or a custom software application, running on a client device, such as a personal computer **218b** including a display **218a**. However, it will be understood that other electronic devices such as personal digital assistants (PDAs), hand-held computers, Internet-ready phones, and WebTVs, may be utilized as client devices for accessing the Web site **212** in accordance with embodiments of the present invention.

The Web server **214** also is configured to communicate with various third parties according to embodiments of the present invention. As will be described below, the Web server **214** is configured to communicate with other users, often referred to as "runners", at runner sites **219**, who perform data entry (Block **110** of Figures 1A-1B and 1D-1E) according to embodiments of the present invention. When using public domain sources, an "Experimental Section" may be the source of data entry as was described above with reference to the Wolfe et al. publication.

Moreover, in other embodiments, data entry may be performed within an entity, such as a corporation or university, using proprietary data that may be contained, for example, in lab notebooks. This can provide institutional memory archiving systems, methods and computer program products that can be used, for example, by large corporations or universities, to archive the results of many chemical synthesis experiments that are contained in lab notebooks. In yet other alternatives, a scientist who is involved in chemical synthesis can archive data that is being generated by the scientist during the course of chemical synthesis. Accordingly, in some embodiments, the customer sites **218** and the runner sites **219** may be combined into a single station.

Finally, the customer sites **218** may communicate with suppliers of chemicals and/or equipment at supplier sites **222**, in performing a transaction **130** of Figures 1A, 1C-1D and 1G, via the Internet **220** and preferably through the Web server **214**. Communications between the customer sites **218**, runner sites **219**, the server Web site **212** and supplier sites **222** are preferably established via the Internet **220**. However, other communication methods and networks may be utilized, including direct-dial access and telephonic communications. Wireless or wire communications may be used.

Referring now to Figure 3, detailed operations for data entry (Block **110** of Figures 1A-1B and 1D-1E) now will be described. As was described above, data entry may be performed by users, also referred to herein as "runners" who may be tasked with a list of target chemicals for which to research public domain synthesis procedures and to enter these procedures in a data entry operation. The target chemicals may be derived from a list of target chemicals that are widely used in industrial and/or academic application. Target chemicals also may be identified based on user queries in a user query operation **120** of Figures 1A-1C and 1F, for which no target chemicals were identified. Other techniques for identifying target chemicals for database entry also may be used. Data entry operations **110** of Figure 3 can facilitate the manual, semiautomatic or automatic entry of narrative procedures, reagent chemicals and equipment that is used to synthesize a target chemical by reacting the reagent chemicals in the equipment according to the procedure.

Referring now to Figure 3, operations begin at Block **310**, where the runner selects a step to modify. Thus, when entering data for a new procedure, Step 1 is selected at Block **312**, for example by selecting the New button of the data entry display of Figure 4.

Referring to Block **314**, the reagents for Step 1 are then entered. As shown in Figure 5, reagents may be entered using a reagent lookup. Alternatively, as shown in Figure 6, reagents may be entered via manual entry.

Then, referring to Block **316**, various properties of the target chemical may be entered by selecting the Properties button of Figure 7 and entering the properties shown at the bottom of Figure 7. As shown, properties can include yield, density, boiling point (BP), flash point (FP), melting point (MP), vapor pressure, Beilstein number, other names and other properties.

At Block **318**, equipment then is entered, for example by manual entry on equipment lists as shown in Figure 8 and/or by equipment lookup as shown in Figure 9. It will be understood that the operations at Blocks **314**, **316** and **318** may be performed in sequences that are different from that illustrated in Figure 3.

Then, referring to Block **330**, the narrative for the first step of the procedure can be generated interactively, for example using the first reagent and the starting equipment, as shown in Figure 10. Figures 11 and 12 illustrate other examples of generation of a step of a procedure by selecting actions, qualifiers, reagents and times using pull-down menus.

Assuming there is another step at Block **332**, the next step may be selected (Block **334**) by selecting the Next button as shown in Figure 13. In particular, to generate the next step at Block **340**, the equipment data is cleared and an action menu may be generated, as shown in Figure 14. At Block **344**, the runner is given the choice of entering the procedure manually or using the drop-down menu. If manually, then at Block **352**, the procedure is typed in manually, and at Block **354**, the reagent is entered from the reagent list by selection. Alternatively, if by drop-down menu, then the actions are selected from the drop-down menu at Block **356**, for example as shown in Figure 14.

For interactive entry, a common template for a procedure step may be provided, such as "into a _____ equipped with _____ is added _____". The runner can then supply the starting flask, equipment list and first reagent using pull-down menus and/or manual entries. The specific quantities may be provided using tags for molar quantities and gram quantities. These quantities may be scaled later, as will be described below.

Returning again to Figure 3, when the last step has been entered at Block **332**, the Save button (Figure 4) may be selected and the data may be stored (Block **336**) in the chemical database **216a** and the equipment database **216b** of Figure 2. In particular, the target chemicals and the reagent chemicals may be stored in the chemical database **216a** that was described in Table 1. The equipment may be entered into the equipment database **216b** that was described in Table 2. Supplier data also may be entered into the supplier database **216c** that was described in Table 3. Supplier data can be entered directly into the database **216c** using the database server **215**, and/or a graphical user interface may be provided to facilitate data entry.

The databases **216a** may be populated as follows: The data may be read from a product data file and may be tab delimited. Complete entries may be separated by a new line. A call is made to a Java servelet located at the server Web site **212**. The servelet accepts a connection and waits for the data. The runner site **219** sends the data and waits for a reply. The servelet at the server Web site **212** reads the data and inserts it into the database **216a** at each new line, using the database server **215**. The entry program also sends the date/time of the last time it updated. The servelet sends any new entries into the database since that time, and all entries in the database are timestamped. The servelet sends the current date/time and the entry program saves it to a file for the next time.

Referring now to Figure 15, additional details for entering properties (Block **316** of Figure 3), according to embodiments of the invention, now will be provided. As shown in Figure 6, the name of the product can be entered in the "Name" field at Block **1510**. The CAS number can be entered into the CAS field of Figure 6 at Block **1512**. Other properties may be entered at Block **1514**. In particular, the formula (Block **1521**) and weight (Block **1522**) may be entered into the appropriate blocks of Figure 6. The boiling point BP (Block **1523**), melting point MP (Block **1524**), Beilstein reference (Block **1525**), vapor pressure (Block **1526**), flash point (Block **1527**) and other names (Block **1528**) may be entered into the appropriate fields of Figure 6. At Block **1532**, the yield also may be entered into the appropriate block of Figure 6. The Reference button of Figure 4 also may be selected, and the reference to the publication where the procedure was obtained may be entered, for example using the pop-up window of Figure 16. Then, at Block **1540**, the information that was entered is saved into the appropriate fields of the chemical database **16a**, for example using the format shown in Table 1 above.

Referring now to Figure 17, operations for performing user queries (Block **120** of Figures 1A-1C and 1F) now will be described in detail. As shown at Block **1710**, a user identification of a target chemical is accepted. At Block **1720**, a listing of reagent chemicals that are used to synthesize the target chemical, a listing of equipment that is used to synthesize the target chemical and a listing of the procedure that is used to synthesize the target chemical by reacting the reagent chemicals in the equipment according to the procedure, is located and displayed.

As shown at Blocks **1721-1726**, many different query techniques may be used to identify a target chemical. In particular, a user identification of a target chemical may be obtained based on CAS number (Block **1721**), chemical name (Block **1722**), chemical formula (Block **1723**) or chemical structure (Block **1726**). Moreover, at Block **1724**, the user identification of a reaction type is accepted and a listing of target chemicals that are synthesized using the reaction type is displayed. Then, a user selection of a target chemical from the listing of target chemicals that are synthesized using the reaction type is accepted. Finally, at Block **1725**, user identification of a keyword may be accepted and a listing of target chemicals that are synthesized using the keyword may be displayed. A user selection of a target chemical from a listing of target chemicals that are synthesized using the keyword then is obtained. Other query techniques also may be used. Based on the input at Blocks **1721-1726**, the locate

operations of Block **1720** perform database searches of the databases **216a-216c** of Figure 2, for example via the database server **215**.

Additional details of the operations of Blocks **1710** and **1720-1726** now will be provided. Figure 18 illustrates an example of a user display that may be displayed at a customer site **218** to accept user input at Block **1710**. As shown in Figure 18, the CAS number, chemical formula or compound name may be entered at field **1810**. Upon entering data at field **1810** and activating the Locate! button, the processing of Block **1720** can first determine whether a valid CAS number is present. If yes, then a search of the databases **216a-216c** may be performed based on the CAS field in Table 1. If a valid CAS number is not present, then a search may be performed on the name and formula fields of Table 1.

A user also may input a chemical structure (Block **1726**) using conventional chemical drawing and/or other drawing programs. The chemical structure then may be searched by converting the chemical structure into an alphanumeric string that represents the chemical structure, for example using conventional conversion tools. For example, the SMILES tool kit, marketed by Daylight Chemical Information Systems, Inc., may be used to convert the chemical structure into an alphanumeric string using protocols that are described at www.daylight.com. In yet another alternative, an MDL tool, marketed by MDL Information Systems, Inc., may be used to convert the chemical structure into an alphanumeric string, as described at www.mdli.com. Other conversion tools may be used. A search then may be performed relative to the smiles and reagent smiles attributes of the chemical database **216a**, as was described in Table 1.

Still referring to Figure 18, alternatively, if the user does not know exactly what the user is searching for, an entry may be made at field **1820** based on reaction type (Block **1724**) or any other keyword (Block **1725**), and the Locate Action Type button can be pressed. A search then is performed on the info, name, equivalent, other_names or other fields of the chemical database **216a**, to attempt to find a match.

Referring now to Block **1730** of Figure 17, a search based on CAS number (Block **1721**), chemical name (Block **1722**) or formula (Block **1723**) may produce a single result of a match or multiple results. If a single result is produced, then the single result is displayed at Block **1740**. However, a search based on reaction type (Block **1724**) or keyword (Block **1725**) generally will provide multiple matches at Block **1730**. If multiple results are present at Block **1730**, a listing of the multiple

results is displayed at Block **1732**. An example of a display of multiple results is shown in Figure 19 based on a search of the chemical name "bromo" in field **1810** of Figure 18. A user selection of one of the matches from the list is then accepted at Block **1734**, and the result is displayed at Block **1740**.

When multiple results are found, a prioritized listing may be displayed, so that more likely desired results are displayed at the top of the listing. In particular, in response to a user input in field **1810** of Figure 18, the name, other_names and info attributes of the chemical database **216a** may be searched. The results may be displayed in a priority sequence as follows: exact matches in the name attribute; exact matches in the other_names attribute; partial matches in the name attribute; and, finally, partial matches in the other_names attribute. By prioritizing the display of results, the more likely user selections may be displayed at the top of the list in Figure 19.

Referring now to Block **1740**, a listing of the reagent chemicals, the corresponding equipment and the corresponding procedure is provided, for example as shown in Figure 20. As shown in Figure 20, the name of the chemical is displayed at **2010**, the reagents are displayed at **2020**, the equipment is displayed at **2030**, the procedure is displayed at **2040**, and the reference that was used to derive the procedure is displayed at **2050**.

The operations of Figure 17 that were described above can facilitate both forward searching and backward searching for target chemicals. In forward searching, a search can be made as to which chemical reactions include a chemical as a reagent. Thus, user identification of a chemical is accepted, and a listing of procedures that use the chemical as a reagent chemical is displayed. A user selection of the procedure from the listing of procedures that use the chemical as a reagent chemical then is accepted. In forward searching, the chemicals attribute of the chemical database **216a** of Table 1 may be searched.

In contrast, in backward searching, a search may be made as to how a target chemical may be synthesized. As was described above, in response to selection of a target chemical, a listing of procedures can be displayed that can be used to synthesize the target chemical. A user selection of the procedure is then accepted. In backward searching, the name attribute of the chemical database **216a** of Table 1 may be searched.

Referring again to Figure 20, the initial display of Figure 20 may default to 0 grams or 0 moles of the reagent chemicals and 0 quantities of the equipment. In order to allow synthesis of a desired amount of the target chemical, the user input of a number of moles of the chemical may be input at field **2060**, as shown at Block **1742**. At Block **1744**, the listings of the reagent chemicals and equipment are scaled, so as to synthesize the desired quantity of the target chemical. Then, at Block **1750**, a scaled listing of reagent chemicals that are used to synthesize the desired quantity of the target chemical, a listing of equipment that is used to synthesize the desired quantity of the target chemical and a listing of a procedure that is used to synthesize the desired quantity of the target chemical is displayed. Figure 21 illustrates a display procedure that includes the desired quantities of reagents and equipment. Referring again to Figure 17, if a customer desires to electronically order the target chemical, reagent chemicals and/or the equipment, the customer proceeds to transaction (Block **130** of Figures 1A, 1C-1D and 1G), as will be described in detail below.

Referring now to Figure 22, additional details of scaling the listings (Block **1744** of Figure 17) now will be described. As shown in Figure 22, the desired quantities may be calculated at the customer site **218** using a browser and/or at the server Web site **212**. In particular, as shown at Block **2210**, if browser side scripting is supported, for example if the browser is JavaScript-capable, then at Block **2220**, the JavaScript method that is specified in the onClick attribute of the Submit button is called. At Block **2230**, this JavaScript method calculates the new values and displays them on the Web page at Block **1750**. It can return false to stop further processing. It also can provide the values to the server Web site **212** as well.

Returning to Block **2210**, if browser side scripting is not supported, then the desired quantity is sent to the server Web site **212** at Block **2240**, for example by calling the Uniform Resource Locator (URL) specified in the action attribute of the form page. The server Web site **212** then calculates the new values at Block **2250** and generates a new HTML page at Block **2250**, which then is sent back to the customer site **218** for display at Block **1750**.

In a specific embodiment, a customer site (client side) JavaScript implementation of the scaler can use the onClick attribute of the HTML tag <input> when the tag also has the attribute type = "submit". An example snippet is as follows:

<form action = http://someplace.com/formhandler>

<input type = "submit" onClick = "return doSomething()">

</form>.

Prior to Netscape Navigator 2.0, the onClick attribute was undefined, so that clicking the Submit button would execute the form action. However, Netscape Navigator 2.0 can cause JavaScript code to be executed prior to calling the action URL defined in the <form>'s action attribute. In Navigator 3.0, the onClick attribute was evaluated for a Boolean (true/false) value. If the value was false, the action URL was not called. Thus, the behavior introduced in Netscape Navigator 3.0 can allow client side only calculation of the scaler value. The calculation can be defined in JavaScript, which is embedded in the HTML page, and referred to this calculation in the onClick attribute.

Referring now to Figure 23, details of performing a transaction (Block **130** of Figures 1A, 1C-1D and 1G) now will be described in detail. In general, user input to order reagent chemicals and/or equipment is accepted and the reagent chemicals and/or equipment are electronically ordered. More specifically, as shown in Block **2310**, a user input is accepted to purchase reagents. The reagents may be purchased individually (Block **2312**) or as a calculated kit (Block **2314**). Moreover, the target chemical itself may be purchased directly from a supplier at Block **2316**. Finally, if a target chemical is not found in the database, but a derivative thereof is found, a request may be sent to bid on the novel derivative at Block **2318**.

Equipment also may be purchased at Block **2320**. The equipment may be purchased individually at Block **2322**, or as a reaction kit at Block **2324**. The supplier database **216c** may be used to electronically request a quote at Block **2325** to the supplier sites **222** over the computer network **220** of Figure 2. A quote then is received at Block **2330**, and, if acceptable, an order is placed at Block **2340**. The order may be placed by communication over the computer network **220** to the supplier sites **222**. A tracking number may be obtained at Block **2350**, and the progress of the order may be monitored at Block **2360**, for example by providing a private Web page that is generated to match the tracking number of Block **2350**. The chemicals and/or equipment then are received at Block **2370**.

In the drawings and specification, there have been disclosed typical preferred embodiments of the invention and, although specific terms are employed, they are used in a generic and descriptive sense only and not for purposes of limitation, the scope of the invention being set forth in the following claims.